

Ab initio studies of fluorinated graphene

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Abstract

Chemisorbed adatoms on graphene might open a crucial control of several properties opening a road to spintronics in graphene. It has been demonstrated that the adatoms can induce magnetic moments [1],[2], controllable spin-orbit coupling [3],[4] as well as wide band gaps [5]. We therefore explore which role fluorine adatoms on graphene could play in this context.

A set of fluorinated graphene unit cells of different sizes and thus different fluorine concentrations were obtained within ab initio calculations using the code WIEN2k [6]. In the talk we present a detailed analysis of the obtained structural parameters. Large binding energies were found indicating strong chemisorption and the stability of fluorinated graphene. Systems with different physical properties (metallic and insulating) were found, pointing to the possibility of modifying the electronic properties of graphene by fluorination. The electronic structure of 1×1 semifluorinated graphene for example is shown in Fig. 1 representing a metallic state. The application of a Bader charge analysis revealed that fluorine adatoms could act as a p-type donor and represent charged impurities.

Different magnetic states are observed in highly fluorinated graphene. In more dilute systems at the stage of 3×3 unit cells magnetic moments start to vanish. Magnetic systems can be obtained with the help of hybrid density functionals by the correction of self interaction errors. A detailed description of the binding of fluorine to graphene in dilute configurations will be given and a proposal of an orbital tight-binding model will be presented. The effects of spin-orbit interaction in fluorinated graphene turn out to be large depending on the fluorine concentration. This is illustrated in Fig. 2 where the absolute band splittings in 1×1 semifluorinated graphene are shown to reach a maximum of 35 meV. Spin-orbit splittings originate from the atomic spin-orbit coupling in fluorine, in contrast to hydrogenated graphene where it is mainly due to sp^3 hybridization [3].

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References

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Figures

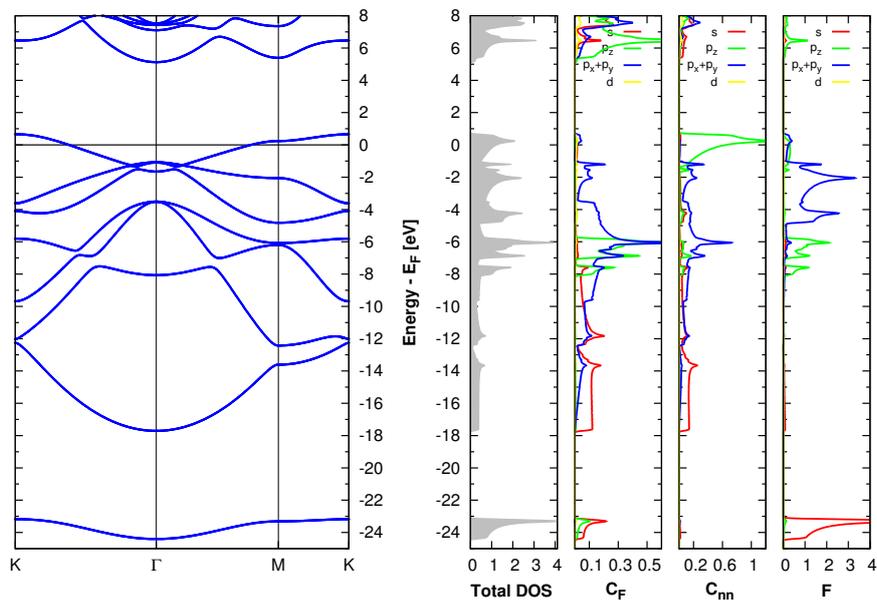


Figure 1: Electronic properties of 1×1 semifluorinated graphene. Left: Non spin polarized band structure representing a metallic state. Right: Orbital resolved density of states describing the bonding in densely fluorinated graphene.

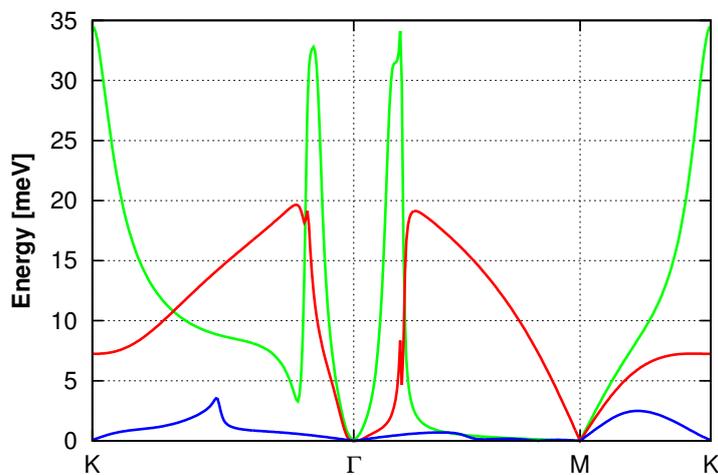


Figure 2: Spin-orbit splittings of the bands in figure 1 around the Fermi energy for 1×1 fluorinated graphene. Valence band splitting (red), the splitting of the band below the valence band (green) and splitting of the conduction band (blue) are shown.